

SN. 09/765425

to overcome 21 Jan 2000

=> search el-e3 sss full

1 104496-04-0/BI
(104496-04-0/RN)
1 125529-39-7/BI
(125529-39-7/RN)
1 528-34-7/BI
(528-34-7/RN)

L8 3 (104496-04-0/BI OR 125529-39-7/BI OR 528-34-7/BI)

=> dis l8 1- sub bib abs

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

L8 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2003 ACS

RN 125529-39-7 REGISTRY

CN 1,2-Cyclobutanedicarboxylic acid, 3,4-bis(4-hydroxyphenyl)-,
(1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,2-Cyclobutanedicarboxylic acid, 3,4-bis(4-hydroxyphenyl)-,
(1.alpha.,2.alpha.,3.beta.,4.beta.)-

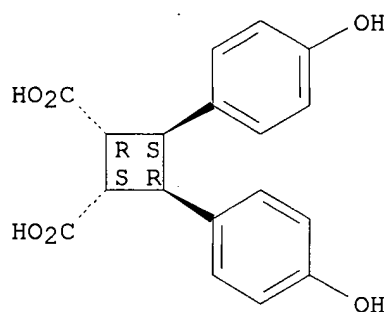
FS STEREOSEARCH

MF C18 H16 O6

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)

2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1

AN 135:117221 CA

TI Diphenylcyclobutane dicarboxylate derivatives as analgesics and
antiinflammatory agents

IN Nakamura, Motoyuki; Yoshizawa, Toyokichi; Chitama, Akira; Nohara,
Toshihiro; Sakurada, Shinobu

PA Showa Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 8 pp.

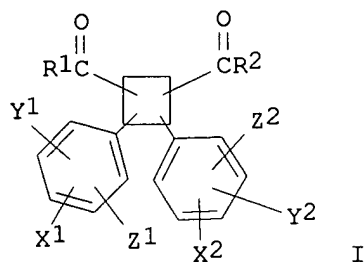
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001199884	A2	20010724	JP 2000-13449	20000121
	EP 1118324	A1	20010725	EP 2001-101213	20010119
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRAI	JP 2000-13449		20000121		
GI					



AB Diphenylcyclobutane dicarboxylate derivs. (I; X1, X2, Y1, Y2, Z1, Z2 = H, OH, halogen, alkyl, alkoxy, N; R1, R2 = OH, halogen, alkoxy, aryloxy, turpenoxy, sugar, N) are claimed as analgesics and antiinflammatory agents with min. toxicity. I were prepd., and their analgesic and antiinflammatory actions and effect on gastric mucosa were tested.

REFERENCE 2

AN 112:115748 CA
 TI Cyclodimers of p-coumaric and ferulic acids in the cell walls of tropical grasses
 AU Ford, Clive W.; Hartley, Roy D.
 CS AFRC Inst. Grassl. Anim. Prod., Hurley/Maidenhead/Berkshire, SL6 5LR, UK
 SO Journal of the Science of Food and Agriculture (1990), 50(1), 29-43
 CODEN: JSFAAE; ISSN: 0022-5142
 DT Journal
 LA English
 AB Cell walls from leaves and stems of three tropical grasses (*Setaria anceps* cv Nandi), pangola grass *Digitaria decumbens*, and spear grass *Heteropogon contortus* were extd. with alkali, and ether-sol. fractions were prepd. from the acidified solns. Cyclobutane dimers derived from p-coumaric acid (CA: 3-(4-hydroxyphenyl) propenoic acid) and ferulic acid (FA: 3-(4-hydroxy-3-methoxyphenyl) propenoic acid) were found in all plant residues. Structural information on the dimers was obtained by gas chromatog.-mass spectrometry. Stem cell wall differed from those of leaves in having major dimer components which contained residues tentatively identified as coniferyl alc. (3-(4-hydroxy-3-methoxyphenyl)-2-propen-1-ol). Species differences in leaf cell wall cyclodimers were evident. Pangola and setaria grasses had dimers mainly derived from FA, whereas spear grass had over 70% of dimers derived from CA. Di-esterification of some dimers in the cell walls was confirmed by the release of dimers contg. the reduced forms of CA and FA (coumaryl and coniferyl alcs. resp.) when leaf cell walls were extd. with borohydride. Heat to tail dimerization giving derivs. of truxillic acid (t-2,c-4-diphenyl-r-1,t-3-cyclobutanedicarboxylic acid) predominated, although evidence was obtained for the presence of head-to-head coumaric acid dimers (derivs. of truxinic acid, t-3,t-4-diphenyl-r-1,c-2-cyclobutanedicarboxylic acid) in setaria stem and spear grass leaf. The results suggested that cyclodimers in grass cell walls occurred in crosslinking structures of varying complexity between macromols., where they would possibly contribute to fiber strength and thus have an adverse effect on the nutritional value of forage.

L8 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2003 ACS

RN 104496-04-0 REGISTRY

CN 1,2-Cyclobutanedicarboxylic acid, 3,4-diphenyl-, bis(4-nitrophenyl) ester, (1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

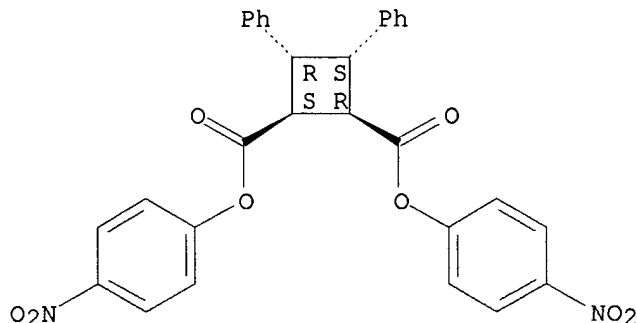
OTHER CA INDEX NAMES:

CN 1,2-Cyclobutanedicarboxylic acid, 3,4-diphenyl-, bis(4-nitrophenyl) ester, (1.alpha.,2.alpha.,3.beta.,4.beta.)-

OTHER NAMES:

CN .beta.-Truxinic acid bis(4-nitrophenyl) ester
 CN Bis(p-nitrophenyl) .beta.-truxinate
 FS STEREOSEARCH
 MF C30 H22 N2 O8
 CI COM
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Relative stereochemistry.



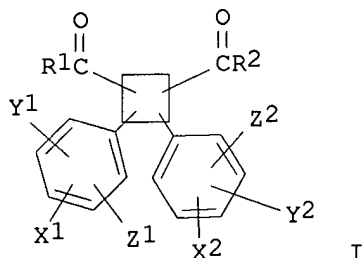
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1962 TO DATE)
 4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1

AN 135:117221 CA
 TI Diphenylcyclobutane dicarboxylate derivatives as analgesics and
 antiinflammatory agents
 IN Nakamura, Motoyuki; Yoshizawa, Toyokichi; Chitama, Akira; Nohara,
 Toshihiro; Sakurada, Shinobu
 PA Showa Pharmaceutical Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001199884	A2	20010724	JP 2000-13449	20000121
	EP 1118324	A1	20010725	EP 2001-101213	20010119
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRAI	JP 2000-13449		20000121		
GI					



AB Diphenylcyclobutane dicarboxylate derivs. (I; X1, X2, Y1, Y2, Z1, Z2 = H,

OH, halogen, alkyl, alkoxy, N; R1, R2 = OH, halogen, alkoxy, aryloxy, turpenoxy, sugar, N) are claimed as analgesics and antiinflammatory agents with min. toxicity. I were prepd., and their analgesic and antiinflammatory actions and effect on gastric mucosa were tested.

REFERENCE 2

AN 110:76172 CA
 TI Polycondensation of bis(p-nitrophenyl) .beta.-truxinate with diamine
 AU Iizawa, Takashi; Miyaji, Takatoshi; Nishikubo, Tadatoshi
 CS Fac. Eng., Kanagawa Univ., Yokohama, 221, Japan
 SO Journal of Polymer Science, Part A: Polymer Chemistry (1988), 26(11), 2941-52
 CODEN: JPACEC; ISSN: 0887-624X
 DT Journal
 LA English
 AB Model reaction of bis(4-nitrophenyl) .beta.-truxinate (I) with aliph. amines proceeded quant. at room temp. Accordingly, polycondensation of I with various diamines was carried out at room temp. or 80.degree.. During the polycondensation with diamines, the pptn. of polymer or gelation of the polymn. soln. occurred, which could limit the mol. wt. of the polymer. On the other hand, the reaction of I with 1,3-bis(4-piperidyl)propane proceeded homogeneously to give a copolymer (II) with relatively high mol. wt., and II showed excellent soly. in many solvents. TG and DTA indicated that the obtained polymers were more stable at lower temps. than around 270.degree.. The polymer prepd. from the polycondensation of I with hexamethylenediamine showed m.p. and decompn. due to imidation at 282.degree.. Photochem. reactions of these polymers were carried out in the film state. Irradn. with 254 nm light caused an absorption at 272 nm to appear and the mol. wt. to decrease. This meant that the scission of cyclobutane rings in the main chain occurred to give cinnamamide structures. The absorption at 272 nm was decreased by irradiation with 302.5 nm light. The UV spectrum of the irradiated polymer differed from that of the original polymer. These results suggested that dimerization of the resulting cinnamamide moieties occurred in competition with their trans-cis-isomerization. On the other hand, the rate of scission of cyclobutane rings of II was faster than that of the corresponding polyamide contg. an .alpha.-truxillamide structure.

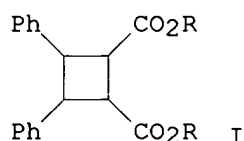
REFERENCE 3

AN 106:66920 CA
 TI Cyclobutane compounds
 IN Nishikubo, Tatatoshi
 PA Research Development Corp. of Japan, Japan
 SO Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF

DT Patent
 LA Japanese
 FAN.CNT 1

102

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 61212532	A2	19860920	JP 1985-53392	19850319
	JP 05088210	B4	19931221		
PRAI	JP 1985-53392		19850319		
GI					

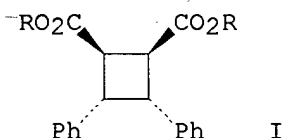


AB Cyclobutane derivs. (I; R = p-O2NC6H4, 4-nitro-1-naphthyl, etc.), useful

as optical materials, are prepd. by photocycloaddn. of PhCH:CHCO₂R (II) in the presence of a dispersant solvent. Thus, 0.059 mol II (R = p-O₂NC₆H₄) in a mixed solvent of 380 mL and 20 mL hexane-MeOH at a dispersion of 20 g/L was irradiated 6 h at 30.degree. with stirring to give 91.2% I (R = p-O₂NC₆H₄).

REFERENCE 4

AN 105:152559 CA
 TI Convenient synthesis of .beta.-truxinic acid via photodimerization of p-nitrophenyl cinnamate in the crystalline state
 AU Nishikubo, Tadatomi; Takahashi, Eiji; Miyaji, Takatoshi; Iizawa, Takashi
 CS Fac. Eng., Kanagawa Univ., Yokohama, 221, Japan
 SO Bulletin of the Chemical Society of Japan (1985), 58(11), 3399-400
 CODEN: BCSJA8; ISSN: 0009-2673
 DT Journal
 LA English
 GI



AB .beta.-Truxinic acid (I, R = H) was prepd. in high yield via topochem. photodimerization of PhCH:CHCO₂C₆H₄NO₂-4 (II) crystals, followed by hydrolysis of the obtained dimer. Thus, II crystals were suspended in hexane under N and irradiated with a 100-W high pressure Hg lamp to give 99.2% I (R = 4-O₂NC₆H₄) which was treated with KOH in MeOH and then concd. HCl to give 96.7% I (R = H).

L8 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2003 ACS

RN **528-34-7** REGISTRY

CN 1,2-Cyclobutanedicarboxylic acid, 3,4-diphenyl-, (1R,2S,3R,4S)-rel- (9CI)
 (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,2-Cyclobutanedicarboxylic acid, 3,4-diphenyl-,
 (1.alpha.,2.alpha.,3.beta.,4.beta.)-

CN 1,2-Cyclobutanedicarboxylic acid, 3,4-diphenyl-, cis-1,2,trans-1,3,trans-1,4- (8CI)

OTHER NAMES:

CN .beta.-Truxinic acid

CN Isotruxillic acid

FS STEREOSEARCH

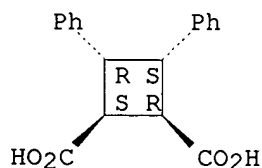
MF C18 H16 O4

CI COM

LC STN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER

(*File contains numerically searchable property data)

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

36 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
36 REFERENCES IN FILE CAPLUS (1962 TO DATE)

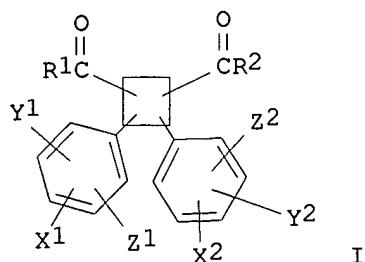
REFERENCE 1

AN 138:39088 CA
TI Topochemical reaction control in solution. III. 4,15-Diamino[2.2]paracyclophane, a reusable template for topochemical reaction control in solution
AU Zitt, Holger; Dix, Ina; Hopf, Henning; Jones, Peter G.
CS Institut fur Organische Chemie, Technische Universitat Braunschweig, Braunschweig, 38106, Germany
SO European Journal of Organic Chemistry (2002), (14), 2298-2307
CODEN: EJOCFK; ISSN: 1434-193X
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
AB An efficient synthesis of [2.2]paracyclophane-4,15-dicarboxylic acid from [2.2]paracyclophane (I) has been developed. The diacid was converted via a diazide into the 4,15-diisocyanato[2.2]paracyclophane (II), a versatile intermediate that could be transformed into many new pseudogeminally substituted derivs. of I. For example, treatment of II with alcs. provided two carbamates. On treatment of II with diisopropylamine, a urea compd., was obtained, whereas redn. with lithium aluminum hydride afforded a cyclic urea (III). Hydrolysis of II furnished a diamine (IV), which was used as a reusable spacer in a [2+2]photoaddn. expt. Thus, treatment of IV with trans-cinnamoyl chloride provided a bis(amide), which on irradiation in acetone ring-closed to give a cyclobutane compd. Sapon. of this yielded 3,4-diphenyl-1,2-cyclobutanedicarboxylic acid (.beta.-truxinic acid) and returned the spacer system 19, both in quant. yield. The X-ray structures of II and III are reported.
RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 135:117221 CA
TI Diphenylcyclobutane dicarboxylate derivatives as analgesics and antiinflammatory agents
IN Nakamura, Motoyuki; Yoshizawa, Toyokichi; Chitama, Akira; Nohara, Toshihiro; Sakurada, Shinobu
PA Showa Pharmaceutical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001199884	A2	20010724	JP 2000-13449	20000121
	EP 1118324	A1	20010725	EP 2001-101213	20010119
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRAI	JP 2000-13449		20000121		
GI					



AB Diphenylcyclobutane dicarboxylate derivs. (I; X1, X2, Y1, Y2, Z1, Z2 = H, OH, halogen, alkyl, alkoxy, N; R1, R2 = OH, halogen, alkoxy, aryloxy, turpenoxy, sugar, N) are claimed as analgesics and antiinflammatory agents with min. toxicity. I were prepd., and their analgesic and antiinflammatory actions and effect on gastric mucosa were tested.

REFERENCE 3

AN 133:321558 CA
 TI Compelled Orientational Control of the Solid-State Photodimerization of trans-Cinnamamides: Dicarboxylic Acid as a Non-covalent Linker
 AU Ito, Y.; Hosomi, H.; Ohba, S.
 CS Graduate School of Engineering, Department of Synthetic Chemistry and Biological Chemistry, Kyoto University, Kyoto, 606-8501, Japan
 SO Tetrahedron (2000), 56(36), 6833-6844
 CODEN: TETRAB; ISSN: 0040-4020
 PB Elsevier Science Ltd.
 DT Journal
 LA English
 AB The 2:1 hydrogen-bonded cocrystals 1a.cntdot.ox, 1a.cntdot.su, 1a.cntdot.pht, 1a.cntdot.fu, 1b.cntdot.ox, 1c.cntdot.ox, 1d.cntdot.ox between 4-R-trans-cinnamamides [1a-11c: R = H, Me, Cl, resp.; 1d = trans-3-(2-thienyl)acrylamide] and dicarboxylic acids (ox, su, gl, fu, pht) were prepd. and characterized by IR and powder X-ray techniques. The crystal structures of 1a.cntdot.pht, 1a.cntdot.ox and 1a.cntdot.fu were solved by single crystal X-ray diffraction. Phthalic acid (pht) caused .beta.-type photodimerization of trans-cinnamamide (1a) in the cocrystal and functioned as a non-covalent linker like gauche 1,2-diamines in photodimerization of trans-cinnamic acids. Oxalic acid (ox) forced 1a to take a bilayer structure that is suitable for .beta.-type photodimerization. In the case of fumaric acid (fu), cross photodimerization with 1a occurred to give a cycloadduct. For the cocrystals 1a.cntdot.pht and 1a.cntdot.fu, pedal-like motion was assumed to occur prior to the dimerization.
 RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 4

AN 129:148662 CA
 TI A controlled photodimerization of cinnamic acid in a composite bilayer of dioctadecyldimethylammonium bromide
 AU Nakamura, Tomotaka; Takagi, Katsuhiko; Sawaki, Yasuhiko
 CS Department of Applied Chemistry, Graduate School of Engineering, Nagoya University, Nagoya, 464-01, Japan
 SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1998), 313, 341-346
 CODEN: MCLCE9; ISSN: 1058-725X
 PB Gordon & Breach Science Publishers
 DT Journal
 LA English
 AB Investigations of the photochem. of cinnamic acid (CA) were carried out in a form of 1: 1 composite solids with dioctadecyldimethylammonium bromide (DODAB) or chloride (DODAC). UV irradiation of the composite solids with DODAB resulted in the highly selective formation of the syn-Head-to-Head

dimer, suggesting the parallel orientation of CA within the complex. Studies of X-ray diffraction, DSC, and IR spectra revealed the formation of a composite bilayer assembly showing the interaction between polar groups of CA and DODAB as well as the incorporation of CA into the alkyl regions of DODAB. On the other hand, the mixt. of CA and DODAC showed less and non-selective photodimerization reaction, which could be ascribed to a disordered mol. arrangement, judging from a weak and broad endothermic peak at around reaction temp. in the DSC curve.

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 5

AN 129:15910 CA
TI Photodimerization of trans-cinnamic acid in a bilayer of dimethyldioctadecylammonium bromide
AU Nakamura, Tomotaka; Takagi, Katsuhiko; Sawaki, Yasuhiko
CS Dep. Applied Chemistry, Fac. Eng., Nagoya Univ., Nagoya, 464-01, Japan
SO Bulletin of the Chemical Society of Japan (1998), 71(4), 909-914
CODEN: BCSJA8; ISSN: 0009-2673
PB Chemical Society of Japan
DT Journal
LA English
AB The photochem. of trans-cinnamic acid (trans-1) was studied in a cast film of dimethyldioctadecylammonium bromide (2), deposited from aq. dispersions as a cryst. solid by the spontaneous vaporization of water. UV irradiation of the cast film resulted in a highly selective formation of the syn-Head-to-Head dimer, suggesting a parallel orientation of trans-1 within a bilayer film. Analyses with X-ray diffraction, differential scanning calorimetry, and IR spectra revealed the formation of a bilayer structure of 2 in which the mols. of trans-1 are dissolved to interact with the polar head groups. The photoreactivity of trans-1 in the cast film was found to be dramatically suppressed by heating at 40-60.degree.C, which is attributed to an improvement in the crystallinity of the bilayer.

RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 6

AN 128:101875 CA
TI Photodimerization of cinnamic acids controlled by molecular assemblies of surfactant amine N-oxides
AU Nakamura, Tomotaka; Takagi, Katsuhiko; Itoh, Mariko; Fujita, Kaori; Katsu, Hiroyuki; Imae, Toyoko; Sawaki, Yasuhiko
CS Dep. Appl. Chem., Fac. Eng., Nagoya Univ., Nagoya, 464-01, Japan
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1997), (12), 2751-2755
CODEN: JCPKBH; ISSN: 0300-9580
PB Royal Society of Chemistry
DT Journal
LA English
AB UV irradiation of (E)-4-RC6H4CH:CHCO2H [I, R = H, OMe] in a complex with surfactant amine N-oxides Me(CH2)nN(O)Me2 (II, n = 11, 13, 15) as vesicles in water leads to the formation of cyclodimers, i.e., .beta.-, .delta.-truxinic and/or .alpha.-truxillic acids. Decreasing the molar ratios of I to II causes the vesicles to transform into rod-like micelles and the yield of the cyclodimers decreases. The addition of HCl or NaOH to aq. solns. of I and II brings about sharp changes in the self-assembly structures from vesicles to micro emulsions or rod-like micelles, accompanied by a change in product distribution in the photolysis of the complex. Upon addition of photoinactive carboxylic acids, phenylpropionic and palmitic acids to the I-Me(CH2)16N(O)Me system, the rod-like micelles change into vesicles by formation of a complex with Me(CH2)16N(O)Me leading to the observation of a diln. effect in the photodimerization upon addition of phenylpropionic acid. However, no diln. effect is observed for palmitic acid. This is found to be attributable to the difference in degrees of mixing of I with the acids in the vesicles. These results show

that photodimerization of I incorporated in II is controlled by a variety of mol. assemblies, i.e. rod-like micelles and homogeneous or heterogeneous vesicles.

RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 7

AN 126:7719 CA
TI Stereoselectivity control of [2 + 2] photocycloaddition by changing site distances of hydrotalcite interlayers
AU Shichi, Tetsuya; Takagi, Katsuhiko; Sawaki, Yasuhiko
CS Fac. Eng., Nagoya Univ., Nagoya, 464-01, Japan
SO Chemical Communications (Cambridge) (1996), (17), 2027-2028
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
AB Stereoselectivity of photocyclodimers of unsatd. carboxylates is shown to be controlled by changing the site distances of clay interlayers.

REFERENCE 8

AN 125:300268 CA
TI Organized photocycloaddition of 4-benzoylbenzoate with unsaturated carboxylates in hydrotalcite clay interlayers
AU Shichi, Tetsuya; Takagi, Katsuhiko; Sawaki, Yusuhiko
CS Dep. of Applied Chem., Nagoya Univ., Nagoya, 464-01, Japan
SO Chemistry Letters (1996), (9), 781-782
CODEN: CMLTAG; ISSN: 0366-7022
PB Nippon Kagakkai
DT Journal
LA English
AB Photoirradn. of a mixt. of 4-benzoylbenzoate (1) and 4-(2-phenylethenyl)benzoate yielded regioselective oxetanes in the presence of hydrotalcite clay. Similar irradiation of a mixt. of 1 and cinnamate gave rise to .beta.-truxinate, but not oxetane. The unexpected formation of oxetanes is understood by the favorable distance between C:O and C:C bonds packed in clay interlayers.

REFERENCE 9

AN 125:33265 CA
TI Photochemical cyclodimerization of cinnamic acids included in surfactant amine oxides
AU Takagi, K.; Nakamura, T.; Katsu, H.; Itoh, M.; Sawaki, Y.; Imae, T.
CS Dep. Appl. Chem., Fac. Eng., Nagoya Univ., Nagoya, 464-01, Japan
SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1996), 277, 495-498
CODEN: MCLCE9; ISSN: 1058-725X
PB Gordon & Breach
DT Journal
LA English
AB Photocyclodimerization of unsubstituted and p-methoxy substituted cinnamic acids incorporated in micelles, vesicles or microemulsions formed by dodecyl- and hexadecyldimethylamine oxides has been studied in water. The dimerization proceeds in vesicles much more efficiently than in micelles with preferable formation of head-to-head dimers. The photoreactivity and the stereochem. of the cyclodimers are affected by structural changes of the mol. aggregates.

REFERENCE 10

AN 124:75179 CA
TI Separation and identification of some monomeric and dimeric phenolic acids by a simple gas chromatographic method using a capillary column and FID-MSD

AU Packert, M.; Steinhart, H.
 CS Inst. Biochemie Lebensmittelchemie, Univ. Hamburg, Hamburg, D-20146,
 Germany
 SO Journal of Chromatographic Science (1995), 33(11), 631-9
 CODEN: JCHSBZ; ISSN: 0021-9665
 PB Preston Publications
 DT Journal
 LA English
 AB The monomeric and dimeric phenolic acids represent highly various
 structural substance classes. Included among the monomers are substituted
 benzoic acid, phenylacetic acid, phenylpropionic acid, and cinnamic acid;
 compds. of the biphenyl and cyclobutane types are representatives of
 dimeric acids. The formation of dimeric acids with a diphenylcyclobutane
 dicarboxylic acid structure from t-p-coumaric acid (t-p-CA) and t-ferulic
 acid (t-FA) via a [2+2]-photocycloaddn. reaction is thoroughly described.
 The products are characterized by using mass spectroscopy and by observing
 their chromatog. behavior. The applied method makes it possible to det.
 over 50 phenolic acid isomers. The following elution sequence for the
 monomeric acids is found: benzoic acids < phenylacetic acids <
 phenylpropionic acids < cinnamic acids. Among the dimeric acids, which
 appeared significantly after the monomeric acids, those with a
 diphenylcyclobutane dicarboxylic acid structure elute before
 cis/trans-dehydrodiferulic acid (c-t-DFA).

=> file ca

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	14.74	318.17

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.86	-1.86

FILE 'CA' ENTERED AT 14:33:04 ON 21 APR 2003
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is
 held by the publishers listed in the PUBLISHER (PB) field (available
 for records published or updated in Chemical Abstracts after December
 26, 1996), unless otherwise indicated in the original publications.
 The CA Lexicon is the copyrighted intellectual property of the
 American Chemical Society and is provided to assist you in searching
 databases on STN. Any dissemination, distribution, copying, or storing
 of this information, without the prior written consent of CAS, is
 strictly prohibited.

FILE COVERS 1907 - 17 Apr 2003 VOL 138 ISS 17
 FILE LAST UPDATED: 17 Apr 2003 (20030417/ED)

This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> search 528-34-7

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
 Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

=> dis l10 1- bib abs

YOU HAVE REQUESTED DATA FROM 36 ANSWERS - CONTINUE? Y/(N):y

L10 ANSWER 1 OF 36 CA COPYRIGHT 2003 ACS

AN 138:39088 CA

TI Topochemical reaction control in solution. III. 4,15-Diamino[2.2]paracyclophane, a reusable template for topochemical reaction control in solution

AU Zitt, Holger; Dix, Ina; Hopf, Henning; Jones, Peter G.

CS Institut fur Organische Chemie, Technische Universitat Braunschweig, Braunschweig, 38106, Germany

SO European Journal of Organic Chemistry (2002), (14), 2298-2307

CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

OS CASREACT 138:39088

AB An efficient synthesis of [2.2]paracyclophane-4,15-dicarboxylic acid from [2.2]paracyclophane (I) has been developed. The diacid was converted via a diazide into the 4,15-diisocyanato[2.2]paracyclophane (II), a versatile intermediate that could be transformed into many new pseudogeminally substituted derivs. of I. For example, treatment of II with alcs. provided two carbamates. On treatment of II with diisopropylamine, a urea compd., was obtained, whereas redn. with lithium aluminum hydride afforded a cyclic urea (III). Hydrolysis of II furnished a diamine (IV), which was used as a reusable spacer in a [2+2]photoaddn. expt. Thus, treatment of IV with trans-cinnamoyl chloride provided a bis(amide), which on irradiation in acetone ring-closed to give a cyclobutane compd. Sapon. of this yielded 3,4-diphenyl-1,2-cyclobutanedicarboxylic acid (.beta.-truxinic acid) and returned the spacer system 19, both in quant. yield. The X-ray structures of II and III are reported.

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 36 CA COPYRIGHT 2003 ACS

AN 135:117221 CA

TI Diphenylcyclobutane dicarboxylate derivatives as analgesics and antiinflammatory agents

IN Nakamura, Motoyuki; Yoshizawa, Toyokichi; Chitama, Akira; Nohara, Toshihiro; Sakurada, Shinobu

PA Showa Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

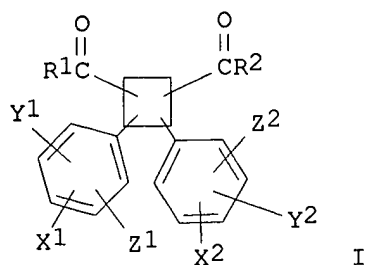
DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001199884	A2	20010724	JP 2000-13449	20000121
	EP 1118324	A1	20010725	EP 2001-101213	20010119
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRAI	JP 2000-13449	A	20000121		

GI



AB Diphenylcyclobutane dicarboxylate derivs. (I; X1, X2, Y1, Y2, Z1, Z2 = H, OH, halogen, alkyl, alkoxy, N; R1, R2 = OH, halogen, alkoxy, aryloxy, turpenoxy, sugar, N) are claimed as analgesics and antiinflammatory agents with min. toxicity. I were prepd., and their analgesic and antiinflammatory actions and effect on gastric mucosa were tested.

L10 ANSWER 3 OF 36 CA COPYRIGHT 2003 ACS

AN 133:321558 CA

TI Compelled Orientational Control of the Solid-State Photodimerization of trans-Cinnamamides: Dicarboxylic Acid as a Non-covalent Linker

AU Ito, Y.; Hosomi, H.; Ohba, S.

CS Graduate School of Engineering, Department of Synthetic Chemistry and Biological Chemistry, Kyoto University, Kyoto, 606-8501, Japan

SO Tetrahedron (2000), 56(36), 6833-6844

CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

AB The 2:1 hydrogen-bonded cocrystals 1a.cntdot.ox, 1a.cntdot.su, 1a.cntdot.pht, 1a.cntdot.fu, 1b.cntdot.ox, 1c.cntdot.ox, 1d.cntdot.ox between 4-R-trans-cinnamamides [1a-11c: R = H, Me, Cl, resp.; 1d = trans-3-(2-thienyl)acrylamide] and dicarboxylic acids (ox, su, gl, fu, pht) were prepd. and characterized by IR and powder X-ray techniques. The crystal structures of 1a.cntdot.pht, 1a.cntdot.ox and 1a.cntdot.fu were solved by single crystal X-ray diffraction. Phthalic acid (pht) caused .beta.-type photodimerization of trans-cinnamamide (1a) in the cocrystal and functioned as a non-covalent linker like gauche 1,2-diamines in photodimerization of trans-cinnamic acids. Oxalic acid (ox) forced 1a to take a bilayer structure that is suitable for .beta.-type photodimerization. In the case of fumaric acid (fu), cross photodimerization with 1a occurred to give a cycloadduct. For the cocrystals 1a.cntdot.pht and 1a.cntdot.fu, pedal-like motion was assumed to occur prior to the dimerization.

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 36 CA COPYRIGHT 2003 ACS

AN 129:148662 CA

TI A controlled photodimerization of cinnamic acid in a composite bilayer of dioctadecyldimethylammonium bromide

AU Nakamura, Tomotaka; Takagi, Katsuhiko; Sawaki, Yasuhiko

CS Department of Applied Chemistry, Graduate School of Engineering, Nagoya University, Nagoya, 464-01, Japan

SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1998), 313, 341-346

CODEN: MCLCE9; ISSN: 1058-725X

PB Gordon & Breach Science Publishers

DT Journal

LA English

AB Investigations of the photochem. of cinnamic acid (CA) were carried out in a form of 1: 1 composite solids with dioctadecyldimethylammonium bromide (DODAB) or chloride (DODAC). UV irradiation of the composite solids with DODAB resulted in the highly selective formation of the syn-Head-to-Head dimer, suggesting the parallel orientation of CA within the complex. Studies of X-ray diffraction, DSC, and IR spectra revealed the formation

of a composite bilayer assembly showing the interaction between polar groups of CA and DODAB as well as the incorporation of CA into the alkyl regions of DODAB. On the other hand, the mixt. of CA and DODAC showed less and non-selective photodimerization reaction, which could be ascribed to a disordered mol. arrangement, judging from a weak and broad endothermic peak at around reaction temp. in the DSC curve.

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 36 CA COPYRIGHT 2003 ACS

AN 129:15910 CA

TI Photodimerization of trans-cinnamic acid in a bilayer of dimethyldioctadecylammonium bromide

AU Nakamura, Tomotaka; Takagi, Katsuhiko; Sawaki, Yasuhiko

CS Dep. Applied Chemistry, Fac. Eng., Nagoya Univ., Nagoya, 464-01, Japan

SO Bulletin of the Chemical Society of Japan (1998), 71(4), 909-914

CODEN: BCSJA8; ISSN: 0009-2673

PB Chemical Society of Japan

DT Journal

LA English

AB The photochem. of trans-cinnamic acid (trans-1) was studied in a cast film of dimethyldioctadecylammonium bromide (2), deposited from aq. dispersions as a cryst. solid by the spontaneous vaporization of water. UV irradiation of the cast film resulted in a highly selective formation of the syn-Head-to-Head dimer, suggesting a parallel orientation of trans-1 within a bilayer film. Analyses with X-ray diffraction, differential scanning calorimetry, and IR spectra revealed the formation of a bilayer structure of 2 in which the mols. of trans-1 are dissolved to interact with the polar head groups. The photoreactivity of trans-1 in the cast film was found to be dramatically suppressed by heating at 40-60.degree.C, which is attributed to an improvement in the crystallinity of the bilayer.

RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 36 CA COPYRIGHT 2003 ACS

AN 128:101875 CA

TI Photodimerization of cinnamic acids controlled by molecular assemblies of surfactant amine N-oxides

AU Nakamura, Tomotaka; Takagi, Katsuhiko; Itoh, Mariko; Fujita, Kaori; Katsu, Hiroyuki; Imae, Toyoko; Sawaki, Yasuhiko

CS Dep. Appl. Chem., Fac. Eng., Nagoya Univ., Nagoya, 464-01, Japan

SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1997), (12), 2751-2755

CODEN: JCPKBH; ISSN: 0300-9580

PB Royal Society of Chemistry

DT Journal

LA English

AB UV irradiation of (E)-4-RC6H4CH:CHCO2H [I, R = H, OMe] in a complex with surfactant amine N-oxides Me(CH2)nN(O)Me2 (II, n = 11, 13, 15) as vesicles in water leads to the formation of cyclodimers, i.e., .beta.-, .delta.-truxinic and/or .alpha.-truxillic acids. Decreasing the molar ratios of I to II causes the vesicles to transform into rod-like micelles and the yield of the cyclodimers decreases. The addition of HCl or NaOH to aq. solns. of I and II brings about sharp changes in the self-assembly structures from vesicles to micro emulsions or rod-like micelles, accompanied by a change in product distribution in the photolysis of the complex. Upon addition of photoinactive carboxylic acids, phenylpropionic and palmitic acids to the I-Me(CH2)16N(O)Me system, the rod-like micelles change into vesicles by formation of a complex with Me(CH2)16N(O)Me leading to the observation of a diln. effect in the photodimerization upon addition of phenylpropionic acid. However, no diln. effect is observed for palmitic acid. This is found to be attributable to the difference in degrees of mixing of I with the acids in the vesicles. These results show that photodimerization of I incorporated in II is controlled by a variety of mol. assemblies, i.e. rod-like micelles and homogeneous or heterogeneous vesicles.

RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L10 ANSWER 7 OF 36 CA COPYRIGHT 2003 ACS
AN 126:7719 CA
TI Stereoselectivity control of [2 + 2] photocycloaddition by changing site distances of hydrotalcite interlayers
AU Shichi, Tetsuya; Takagi, Katsuhiko; Sawaki, Yasuhiko
CS Fac. Eng., Nagoya Univ., Nagoya, 464-01, Japan
SO Chemical Communications (Cambridge) (1996), (17), 2027-2028
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
AB Stereoselectivity of photocyclodimers of unsatd. carboxylates is shown to be controlled by changing the site distances of clay interlayers.
- L10 ANSWER 8 OF 36 CA COPYRIGHT 2003 ACS
AN 125:300268 CA
TI Organized photocycloaddition of 4-benzoylbenzoate with unsaturated carboxylates in hydrotalcite clay interlayers
AU Shichi, Tetsuya; Takagi, Katsuhiko; Sawaki, Yusuhiko
CS Dep. of Applied Chem., Nagoya Univ., Nagoya, 464-01, Japan
SO Chemistry Letters (1996), (9), 781-782
CODEN: CMLTAG; ISSN: 0366-7022
PB Nippon Kagakkai
DT Journal
LA English
AB Photoirradn. of a mixt. of 4-benzoylbenzoate (1) and 4-(2-phenylethenyl)benzoate yielded regioselective oxetanes in the presence of hydrotalcite clay. Similar irradiation of a mixt. of 1 and cinnamate gave rise to .beta.-truxinate, but not oxetane. The unexpected formation of oxetanes is understood by the favorable distance between C:O and C:C bonds packed in clay interlayers.
- L10 ANSWER 9 OF 36 CA COPYRIGHT 2003 ACS
AN 125:33265 CA
TI Photochemical cyclodimerization of cinnamic acids included in surfactant amine oxides
AU Takagi, K.; Nakamura, T.; Katsu, H.; Itoh, M.; Sawaki, Y.; Imae, T.
CS Dep. Appl. Chem., Fac. Eng., Nagoya Univ., Nagoya, 464-01, Japan
SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1996), 277, 495-498
CODEN: MCLCE9; ISSN: 1058-725X
PB Gordon & Breach
DT Journal
LA English
AB Photocyclodimerization of unsubstituted and p-methoxy substituted cinnamic acids incorporated in micelles, vesicles or microemulsions formed by dodecyl- and hexadecyldimethylamine oxides has been studied in water. The dimerization proceeds in vesicles much more efficiently than in micelles with preferable formation of head-to-head dimers. The photoreactivity and the stereochem. of the cyclodimers are affected by structural changes of the mol. aggregates.
- L10 ANSWER 10 OF 36 CA COPYRIGHT 2003 ACS
AN 124:75179 CA
TI Separation and identification of some monomeric and dimeric phenolic acids by a simple gas chromatographic method using a capillary column and FID-MSD
AU Packert, M.; Steinhart, H.
CS Inst. Biochemie Lebensmittelchemie, Univ. Hamburg, Hamburg, D-20146, Germany
SO Journal of Chromatographic Science (1995), 33(11), 631-9
CODEN: JCHSBZ; ISSN: 0021-9665
PB Preston Publications
DT Journal
LA English

AB The monomeric and dimeric phenolic acids represent highly various structural substance classes. Included among the monomers are substituted benzoic acid, phenylacetic acid, phenylpropionic acid, and cinnamic acid; compds. of the biphenyl and cyclobutane types are representatives of dimeric acids. The formation of dimeric acids with a diphenylcyclobutane dicarboxylic acid structure from t-p-coumaric acid (t-p-CA) and t-ferulic acid (t-FA) via a [2+2]-photocycloaddn. reaction is thoroughly described. The products are characterized by using mass spectroscopy and by observing their chromatog. behavior. The applied method makes it possible to det. over 50 phenolic acid isomers. The following elution sequence for the monomeric acids is found: benzoic acids < phenylacetic acids < phenylpropionic acids < cinnamic acids. Among the dimeric acids, which appeared significantly after the monomeric acids, those with a diphenylcyclobutane dicarboxylic acid structure elute before cis/trans-dehydrodiferulic acid (c-t-DFA).

L10 ANSWER 11 OF 36 CA COPYRIGHT 2003 ACS

AN 123:338809 CA

TI Control of solid-state photodimerization of trans-cinnamic acid by double salt formation with diamines

AU Ito, Yoshikatsu; Borecka, Bozena; Trotter, Majes; Scheffer, John R.

CS Fac. Eng., Kyoto Univ., Kyoto, 606, Japan

SO Tetrahedron Letters (1995), 36(34), 6083-6

CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier

DT Journal

LA English

AB By double salt formation, diamines can steer the solid-state [2+2] photodimerization of trans-cinnamic acid (1). Thus, the yields for the photodimerization were significant only in three double salts, i.e., the ones with 1,3-propanediamine and trans- and cis-1,2-cyclohexanediamine, which are assumed to have an overlap structure. The result photodimer is generally .beta.-truxinic acid although in one case, .epsilon.-truxillic acid was formed. .alpha.-Truxillic acid was not produced from any of the double salts studied. The X-ray crystal structures of three double salts of low photoreactivity (1.cntdot.ethylenediamine, 1.cntdot.1,2-propanediamine, 1.cntdot.1,6-hexanediamine) were consistent with Schmidt's rule.

L10 ANSWER 12 OF 36 CA COPYRIGHT 2003 ACS

AN 122:326222 CA

TI Photocyclodimerization of Cinnamic Acid on a Reaction Matrix: Structural Effect of Molecular Assemblies Constructed by Amphiphilic Compounds

AU Imae, Toyoko; Tsubota, Toshinari; Mori, Osamu; Takagi, Katsuhiko; Itoh, Mariko; Sawaki, Yasuhiko

CS Department of Chemistry, Faculty of Science, Chikusa, 464, Japan

SO Journal of Physical Chemistry (1995), 99(16), 6046-53

CODEN: JPCHAX; ISSN: 0022-3654

PB American Chemical Society

DT Journal

LA English

AB Light scattering measurement, video-enhanced differential interference microscopic and electron microscopic observations, ¹H-NMR measurement, and photocyclodimerization were carried out for aq. solns. of alkyl dimethylamine oxides (C12DAO and C16DAO) and dioctadecyldimethylammonium chloride (2C18DAC) with addn. of cinnamic acid. Mol. assemblies in CnDAO:cinnamic acid solns. were converted from micelles to vesicles with increasing mixing ratios of cinnamic acid, while 2C18DAC in water always formed vesicles with addn. of cinnamic acid. Structural changes in reaction matrixes and mol. assemblies constructed by amphiphilic compds. were reflected in the reactivity and stereochem. selectivity of photocyclodimerization. It was concluded that the photodimerization proceeded effectively in vesicles rather than in micelles. The dimerization yields increased with mixing ratio and were in the order of syn-HT < syn-HH < anti-HH (where HT represents head-to-tail and HH represents head-to-head). The product selectivity was discussed in relation to the arrangement of cinnamic acid on mol. assemblies.

L10 ANSWER 13 OF 36 CA COPYRIGHT 2003 ACS

AN 122:150816 CA

TI .epsilon.-PMTC, an opioid antagonist bivalent ligand based on
N-(phenylpropyl)normetazocine with very high preference for .mu. sites
AU Ronsisvalle, Giuseppe; Pappalardo, Maria S.; Prezzavento, Orazio;
Marrazzo, Agostino; Caccamese, Salvatore; Carboni, Lucia; Spampinato,
Santi

CS Istituto di Chimica Farmaceutica e Tossicologica, Universita degli Studi
di Catania, Catania, 95125, Italy

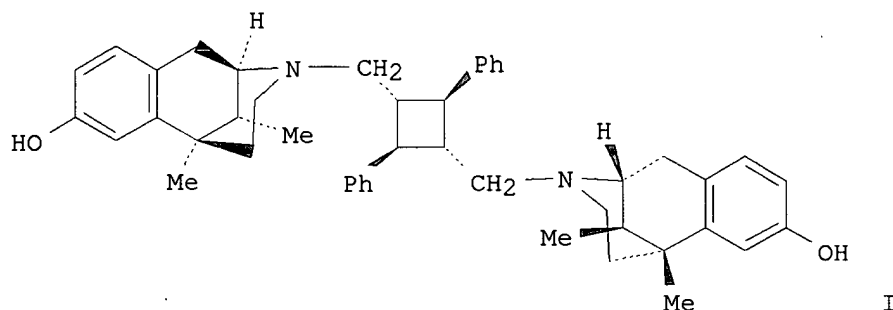
SO Medicinal Chemistry Research (1994), 4(4), 245-53
CODEN: MCREEB; ISSN: 1054-2523

PB Birkhaeuser

DT Journal

LA English

GI



AB The synthesis and opioid receptor affinity of three rigid isomeric bivalent ligands consisting of a cyclobutane matrix that supports two pharmacophoric units derived from benzomorphan are described. The bivalent ligand cis-1,3-bis[3-(6,11-dimethyl-1,2,3,4,5,6-hexahydro-2,6-methano-8-hydroxy-3-benzazocinyl)methyl]-cis-2,4-diphenylcyclobutane, (I .epsilon.-PMTC) displayed selective binding affinity toward .mu. opioid receptors and antagonist character in both in vivo and in vitro assays.

L10 ANSWER 14 OF 36 CA COPYRIGHT 2003 ACS

AN 121:267525 CA

TI Aggregate Formation and Photoreactivity in Phospholipid Vesicles and Langmuir-Blodgett Multilayers: Topologically Controlled Photodimerization of Amphiphilic Styrenes

AU Zhao, Xiao-Mei; Perlstein, Jerome; Whitten, David G.

CS Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA

SO Journal of the American Chemical Society (1994), 116(23), 10463-7
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

AB The amphiphilic styrene fatty acid (I) and its corresponding phosphatidylcholine deriv. (II) have been found to exhibit aggregate formation and topol. controlled photodimerization in Langmuir-Blodgett (LB) assemblies and phospholipid vesicles, resp. For both compds., formation of the .beta. or syn, head-to-head photodimer is the chief photoreaction obsd. upon irradiation. in the assemblies; a trace of the cis styrene is obsd. on irradiation. in the phospholipid vesicles. Changes in the absorption spectrum and a lack of fluorescence in the assemblies, compared to dil. org. solns., suggest that I and II exist as "H" aggregates in both the LB films and vesicles. Monte Carlo simulations suggest that the most stable structure in a monolayer is a simple translation aggregate. Energy minimization gives a cross sectional area in good agreement with that measured for films at the air-water interface. The calcd. structure has nearest neighbor separation within the "magic distance" for solid state

photodimerization of 4.10 .ANG.. The relatively small calcd. tilt angle suggests that dimers can be formed without substantial reorganization. The .lambda.max for the aggregate estd. by an extended dipole calcn. shows good agreement with the measured absorption max. Vesicles of II, either pure or with excess satd. phospholipid, give topol. controlled formation of the .beta. dimer via photolysis of an aggregated form.

L10 ANSWER 15 OF 36 CA COPYRIGHT 2003 ACS

AN 120:263170 CA

TI The anatomy of a cocaine comparison case: a prosecutorial and chemistry perspective

AU Moore, James M.; Meyers, Richard P.; Jimenez, Marcos D.

CS Spec. Test. Res. Lab., U.S. Drug Enforcement Adm., McLean, VA, USA

SO Journal of Forensic Sciences (1993), 38(6), 1305-25

CODEN: JFSCAS; ISSN: 0022-1198

DT Journal

LA English

AB Methodol. used for the comparative chem. analyses of two illicit cocaine seizures, and its application in a successful criminal prosecution, is described. A description of events leading to the arrest of the defendant and an overview of the jury trial are provided. Illicit cocaine, found in the defendant's suitcase and wallet, was subjected to chem. derivatization and three distinct gas chromatog. methods for the detection and relative quantitation of cocaine manufg. impurities/byproducts. The cocaine impurities included cis- and trans-cinnamoylcocaine, the isomeric truxillines and the hydroxycocaines. Among the cocaine manufg. byproducts detected were benzoylecgonine, ecgonine Me ester, ecgonine, N-benzoylnorecgonine Me ester and N-norcocaine. Chem. derivatization of the cocaine samples was accomplished using heptafluorobutyric anhydride and N,O-bis(trimethylsilyl)acetamide. The derivatized impurities/byproducts were subjected to capillary gas chromatog. anal. using both flame ionization and electron-capture detectors. The comparative chem. analyses provided a pos. correlation between the suitcase and wallet cocaine samples.

L10 ANSWER 16 OF 36 CA COPYRIGHT 2003 ACS

AN 118:124269 CA

TI Synthesis of a 7,7'-cyclolignane and a 7',8'-cyclo-7,8'-neolignane via photodimerization of (E)-cinnamic acids in the solid state

AU Fonseca, Sebastiao F.; Rossi, Eleonilce Rosa B.

CS Inst. Quim., Univ. Estadual Campinas, Campinas, 13081, Brazil

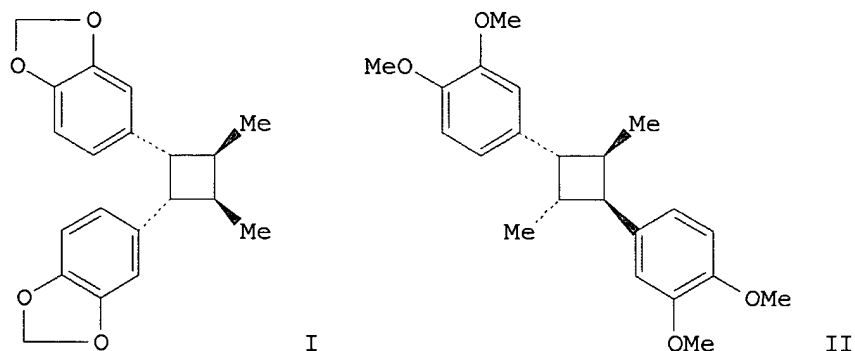
SO Journal of Chemical Research, Synopses (1992), (12), 406-7

CODEN: JRPSDC; ISSN: 0308-2342

DT Journal

LA English

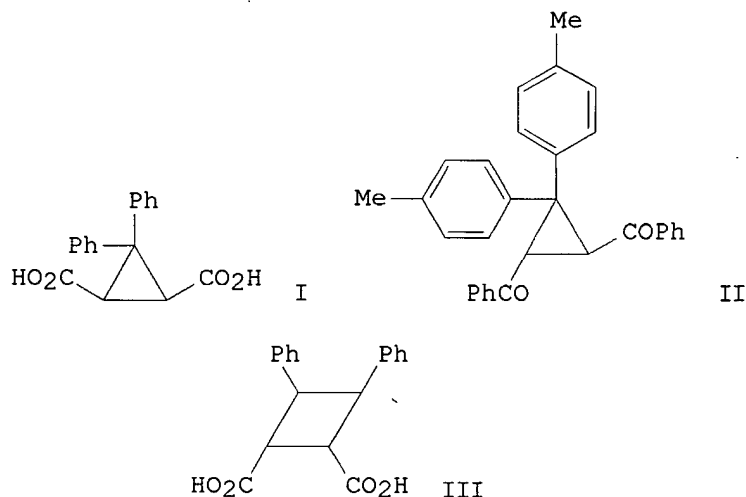
GI



AB The photodimerizations of (E)-3,4-RR1C6H3CH:CHCO2H (R,R1 = methylenedioxy, R = R1 = MeO) in the solid state, followed by a short sequence of transformations, afforded 7,7'-cyclolignane I and 7',8'-cyclo-7,8'-neolignane II resp.

L10 ANSWER 17 OF 36 CA COPYRIGHT 2003 ACS
 AN 116:214025 CA
 TI Stereocontrolled photochemical [2 + 2] cycloaddition
 AU Fleming, Steven A.; Ward, Susan C.
 CS Dep. Chem., Brigham Young Univ., Provo, UT, 84602, USA
 SO Tetrahedron Letters (1992), 33(8), 1013-16
 CODEN: TELEAY; ISSN: 0040-4039
 DT Journal
 LA English
 OS CASREACT 116:214025
 AB Siloxanes were used as tethers in photochem. [2+2] reactions. Dicinnyldimethylsiloxane and dicinnyldiphenylsiloxane were prepd. from cinnamyl alc. and the resp. silanes. After photolysis only one cyclobutane product, the all trans isomer, was obsd. in nearly quant. yield. Titanium as tether gave very low conversions.

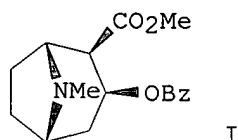
L10 ANSWER 18 OF 36 CA COPYRIGHT 2003 ACS
 AN 111:194131 CA
 TI New host family based on small-ring compounds
 AU Weber, Edwin; Hecker, Manfred; Csoeregh, Ingeborg; Czugler, Matyas
 CS Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300/1, Fed. Rep. Ger.
 SO Journal of the American Chemical Society (1989), 111(20), 7866-72
 CODEN: JACSAT; ISSN: 0002-7863
 DT Journal
 LA English
 OS CASREACT 111:194131
 GI



AB Three- and four-membered ring compds. with functional groups and bulky substituents, e.g., I, II and III, have proved to be a rewarding new source of inclusion hosts. These hosts form inclusion complexes with a variety of uncharged org. mols. ranging from protic dipolar to apolar compds. (168 different inclusion species). Formation and selectivity depend in a systematic manner on structural parameters of the host, such as the nature, no., and position of functional groups, the substituents, and ring size. X-ray structure analyses of I, I.Me₃COH and II.MeCN are reported, revealing the building principles of the new clathrate family. The structures exhibit linear chains of inter-/intramol. H-bridges between carboxylic groups in the free host I and H-bridge aggregation of host and guest mols. in infinite helical chains for the I.Me₃COH (1:1) inclusion. In II.MeCN (1:1), the guest mols. are tightly enclosed by the host framework without further specific interactions.

L10 ANSWER 19 OF 36 CA COPYRIGHT 2003 ACS
 AN 110:23458 CA
 TI Regioselective photodimerization of cinnamic acid in a micellar solution
 AU Nakamura, Yushin
 CS Fac. Pharm. Sci., Josai Univ., Sakado, 350-02, Japan
 SO Journal of the Chemical Society, Chemical Communications (1988), (7),
 477-8
 CODEN: JCCCAT; ISSN: 0022-4936
 DT Journal
 LA English
 AB Irradn. of trans-cinnamic acid (I) and its Me ester (II) in 1% aq. CTAB
 gave dimeric products in 35 and 29% yields as a mixt. of truxinic and
 truxillic acids in a ratio of 19:1 and 3.8:1, resp., while in homogeneous
 solns. I gave no photodimers and II gave dimeric products in 2.3% yield
 under similar reaction conditions.

L10 ANSWER 20 OF 36 CA COPYRIGHT 2003 ACS
 AN 107:192404 CA
 TI Analysis of manufacturing by-products and impurities in illicit cocaine
 via high-performance liquid chromatography and photodiode array detection
 AU Lurie, I. S.; Moore, J. M.; Cooper, D. A.; Kram, T. C.
 CS Spec. Test. Res. Lab., Drug Enforc. Adm., McLean, VA, 22102, USA
 SO Journal of Chromatography (1987), 405, 273-81
 CODEN: JOCRAM; ISSN: 0021-9673
 DT Journal
 LA English
 GI



AB An HPLC method is reported for the detection of manufg. byproducts and
 impurities in illicitly produced cocaine (I). For the 1st time,
 peak-enriched chromatograms were obtained using HPLC, and were
 accomplished using reversed-phase chromatog. and photodiode array
 detection. The use of SDS as an ion-pairing reagent permitted the
 simultaneous sepn. of acids, monoprotic amines, and diprotic amines, and,
 in combination with gradient elution, greatly increased the no. of compds.
 sepd. A mixed binary-ternary gradient was used to further optimize the
 sepn. Dual UV detection at 215 and 277 nm was used. The chromatogram at
 215 nm consisted 1st of carboxylic acids such as benzoic acid, cinnamic
 acid (cis and trans), and several isomers of truxillic and truxinic acid;
 next, the monoprotic amines benzoylecgonine and cinnamoylcocaine (cis and
 trans); and last a group of compds. which are believed to be isomers of
 the diprotic amine truxilline. In addn., simultaneous detection at 277 nm
 permitted the selective detection of various compds., some of which are
 addnl. components. The rapid acquisition of UV spectra greatly
 facilitated compd. identification.

L10 ANSWER 21 OF 36 CA COPYRIGHT 2003 ACS
 AN 107:153689 CA
 TI Organic photochemical reactions. 81. Conrotatory electrocycloreversion
 of cis-3,4-diarylcyclobutene cation radical
 AU Miyashi, Tsutomu; Wakamatsu, Kan; Akiya, Teruhiko; Kikuchi, Koichi; Mukai,
 Toshio
 CS Fac. Sci., Tohoku Univ., Sendai, 980, Japan
 SO Journal of the American Chemical Society (1987), 109(17), 5270-1
 CODEN: JACSAT; ISSN: 0002-7863
 DT Journal

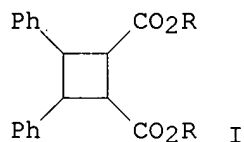
LA English
 OS CASREACT 107:153689
 AB In order to test theor. predications for a stereochem. course of the electrocycloreversion reaction of a cyclobutene radical cation to a 1,3-butadiene radical cation, photochem. electron-transfer reactions of cis-3,4-diarylcyclobutenes were investigated. Cis-3,4-Diarylcyclobutene radical cations generated either by the photoexcitation of the electron donor-acceptor complexes with TCNE or under the 2,6,9,10-tetracyanoanthracene-sensitized conditions efficiently isomerized to cis,trans-1,4-diaryl-1,3-butadienes, demonstrating the occurrence of the stereospecific conrotatory electrocycloreversion.

L10 ANSWER 22 OF 36 CA COPYRIGHT 2003 ACS
 AN 106:66920 CA
 TI Cyclobutane compounds
 IN Nishikubo, Tatatomi
 PA Research Development Corp. of Japan, Japan
 SO Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF

DT Patent
 LA Japanese

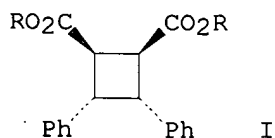
FAN CNT 1

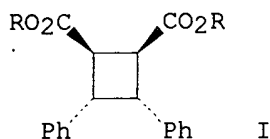
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 61212532	A2	19860920	JP 1985-53392	19850319
	JP 05088210	B4	19931221		
PRAI	JP 1985-53392		19850319		
OS	CASREACT 106:66920				
GI					



AB Cyclobutane derivs. (I; R = p-O₂NC₆H₄, 4-nitro-1-naphthyl, etc.), useful as optical materials, are prepd. by photocycloaddn. of PhCH:CHCO₂R (II) in the presence of a dispersant solvent. Thus, 0.059 mol II (R = p-O₂NC₆H₄) in a mixed solvent of 380 mL and 20 mL hexane-MeOH at a dispersion of 20 g/L was irradiated 6 h at 30.degree. with stirring to give 91.2% I (R = p-O₂NC₆H₄).

L10 ANSWER 23 OF 36 CA COPYRIGHT 2003 ACS
 AN 105:152559 CA
 TI Convenient synthesis of .beta.-truxinic acid via photodimerization of p-nitrophenyl cinnamate in the crystalline state
 AU Nishikubo, Tadatomi; Takahashi, Eiji; Miyaji, Takatoshi; Iizawa, Takashi
 CS Fac. Eng., Kanagawa Univ., Yokohama, 221, Japan
 SO Bulletin of the Chemical Society of Japan (1985), 58(11), 3399-400
 CODEN: BCSJA8; ISSN: 0009-2673
 DT Journal
 LA English
 OS CASREACT 105:152559
 GI





AB .beta.-Truxinic acid (I, R = H) was prepd. in high yield via topochem. photodimerization of PhCH:CHCO₂C₆H₄NO₂-4 (II) crystals, followed by hydrolysis of the obtained dimer. Thus, II crystals were suspended in hexane under N and irradiated with a 100-W high pressure Hg lamp to give 99.2% I (R = 4-O₂NC₆H₄) which was treated with KOH in MeOH and then concd. HCl to give 96.7% I (R = H).

L10 ANSWER 24 OF 36 CA COPYRIGHT 2003 ACS

AN 103:203595 CA

TI Application of anisotropic photocleavage of head-to-head type cyclobutane compounds

AU Yonezawa, Noriyuki; Yamashita, Takashi; Kanoe, Toshio; Saigo, Kazuhiko; Hasegawa, Masaki

CS Fac. Eng., Univ. Tokyo, Tokyo, 113, Japan

SO Industrial & Engineering Chemistry Product Research and Development (1985), 24(4), 593-8

CODEN: IEPRA6; ISSN: 0196-4321

DT Journal

LA English

AB The cyclobutane ring in head-to-head coumarin dimers and their lactone-opened derivs. photocleaves in 3 different modes: sym., asym., and competitive. On the basis of the structural factors governing these pathways, controlling the mode of the photocleavage reaction of some head-to-head cyclobutane compds. was put into practice. The polyamide derived from coumarin dimer was transformed to another linear polyamide by exclusively asym. photocleavage of the cyclobutane rings in the main chain. The pH of a soln. contg. monoanilide derivs. of coumarin dimer was changed by photoirradn. due to the cleavage of the cyclobutane ring followed by spontaneous relactonization. An unsym. substituted stilbene was synthesized from a substituted cinnamic anhydride by intramol. photocycloaddn. and asym. photocleavage.

L10 ANSWER 25 OF 36 CA COPYRIGHT 2003 ACS

AN 102:45264 CA

TI Luminescence and photolytic cycloreversion of cyclobutane derivatives: cinnamic acid dimers and their diamides

AU Aloisi, Gian Gaetano; Mazzucato, Ugo; Bartocci, Giampiero; Cavicchio, Giancarlo; Maravigna, Pietro; Montaudo, Giorgio

CS Dip. Chim., Univ. Perugia, Perugia, I-06100, Italy

SO Zeitschrift fuer Physikalische Chemie (Muenchen, Germany) (1983), 138(2), 207-21

CODEN: ZPCFAX; ISSN: 0044-3336

DT Journal

LA English

AB The fluorescence and photocycloreversion quantum yields for four cinnamic acid dimers and their diamides have been detd. in acetonitrile and methanol and their decay rate parameters estd. The results emphasize that the deactivation of the excited dimers occurs mainly through radiationless paths different from the photochem. cleavage reaction. The corresponding diamides have been also studied in water-methanol solns. at different pH. The trend of the fluorescence and photoreaction quantum yield as a function of pH gives information on the role of the acid-base equil. in the excited state on the photocleavage process.

L10 ANSWER 26 OF 36 CA COPYRIGHT 2003 ACS

AN 93:150844 CA

TI Photodegradation of polyamides and model diamides containing photoreactive truxillic units

AU Aloisi, Gian Gaetano; Mazzucato, Ugo; Maravigna, Pietro; Montaudo,

Giorgio; Recca, Antonio; Scamporrino, Emilio
CS Dip. Chim., Univ. Perugia, Perugia, Italy
SO Chimica e l'Industria (Milan, Italy) (1979), 61(11), 800-5
CODEN: CINMAB; ISSN: 0009-4315
DT Journal
LA English
AB The photodegrdn. of polyamides and diamides of truxillic acid (I) and truxinic acid was studied by viscometry and spectrophotometry. In copolyamides of I and adipic acid, a relatively low I content gives a marked increase in the photolysis rate. The presence of strong acids increases the quantum yield from I derivs. (.alpha. and .epsilon. isomers) noticeably. The similarity of plots of fluorescence and photolysis vs. pH indicates that protonation in the 1st excited singlet state favors ring cleavage of these isomers. Photosensitization to shift the excitation spectrum of photolysis towards the visible region was studied.

L10 ANSWER 27 OF 36 CA COPYRIGHT 2003 ACS

AN 92:216000 CA

TI Stereoselective syntheses via a photochemical template effect

AU Damen, Julien; Neckers, D. C.

CS Dep. Chem., Bowling Green State Univ., Bowling Green, OH, 43403, USA

SO Journal of the American Chemical Society (1980), 102(9), 3265-7

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

AB Bis(vinylbenzyl) truxillate-divinylbenzene-styrene copolymers (I) were hydrolyzed, the polymer alcs. were esterified with trans-cinnamoyl chloride and UV-irradiated in C6H6 suspension, and the resulting photodimers were liberated by acid hydrolysis. The polymer matrix directed the dimerization to occur >50% of the time in a stereochem. direction which did not occur at all in monomers or in random polymer analogs. Irradn. of the trans-cinnamate of hydrolyzed I prepd. with .beta.-truxinic acid (II) [528-34-7] vinylbenzyl ester, for example, gave 53% II, although the cinnamate of hydrolyzed random I gave only the .alpha.-isomer.

L10 ANSWER 28 OF 36 CA COPYRIGHT 2003 ACS

AN 88:112479 CA

TI Cathodic reduction of derivatives of dibenzylidenesuccinic acid; attempted electrohydrocyclization of conjugated systems

AU Andersson, Jan; Eberson, Lennart

CS Chem. Cent., Univ. Lund, Lund, Swed.

SO Nouveau Journal de Chimie (1977), 1(5), 413-18

CODEN: NJCHD4; ISSN: 0398-9836

DT Journal

LA English

AB Bisactivated conjugated diolefins, in the form of the (E,E) and (Z,Z) forms of dibenzylidenesuccinic acid and the (E,E) isomer of its N-methylimide, were reduced at a Hg cathode. The expected cyclobutane derivs. (di-Me truxinates and its N-methylimide) were however not formed; instead products of double bond satn., (derivs. of benzylbenzylidene as well as 2,3-dibenzylsuccinic acid) were isolated.

L10 ANSWER 29 OF 36 CA COPYRIGHT 2003 ACS

AN 86:16321 CA

TI Solid state photodimerization of surfactant esters of cinnamic acid

AU Bolt, John; Quina, Frank H.; Whitten, David G.

CS Dep. Chem., Univ. North Carolina, Chapel Hill, NC, USA ✓

SO Tetrahedron Letters (1976), (30), 2595-8

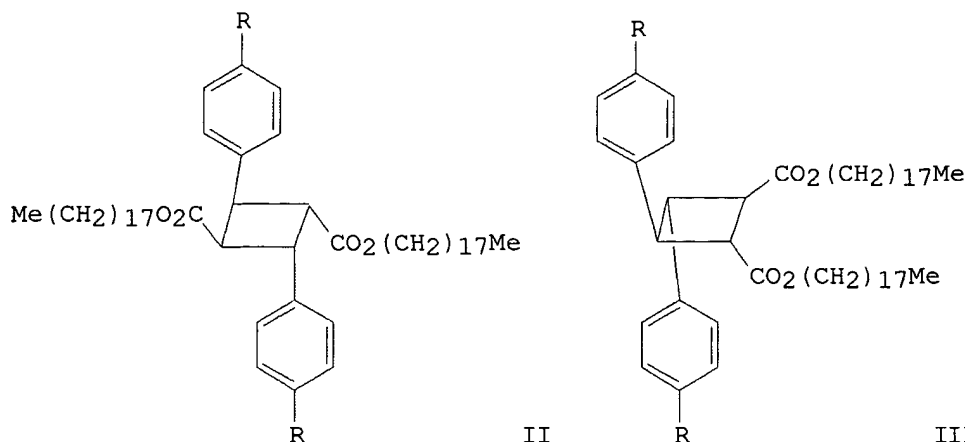
CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

GI

QD 241 T42



AB Octadecyl trans-cinnamate (I) on crystn. from several solvents under various conditions gave 3 different crystal forms. Form A, prepd. by slow crystn. from alcs. or by concg. solns. of I in hydrocarbon or chlorocarbon solvents, on irradiation dimerized to the diester II (R = H). Form B, obtained by crystn. of I from ketonic solvents, was photostable. Form C, obtained by rapid cooling of EtOH solns. of I, on irradiation dimerized to the diester III (R = H). Similarly, octadecyl trans-p-chlorocinnamate (IV) provided 2 crystal forms. Recrystn. of IV from Me₂CO gave photostable crystals. Crystals obtained from 5:1 EtOH-C₆H₆ dimerized on irradiation to the diester II (R = Cl). Irradiation of IV at approx. 40 degree. gave a mixture of II and III (R = Cl).

L10 ANSWER 30 OF 36 CA COPYRIGHT 2003 ACS

AN 82:155084 CA

TI Photodimers of cinnamic acid and related compounds. Stereochemical study of NMR

AU Montaudo, G.; Caccamese, S.; Librando, V.

CS Inst. Ind. Chem., Univ. Catania, Catania, Italy

SO Organic Magnetic Resonance (1974), 6(10), 534-6

CODEN: ORMRBD; ISSN: 0030-4921

DT Journal

LA English

AB The NMR spectra of photodimers of cinnamic acid, chalcone, and 9 related compounds were analyzed and all coupling constants obtained. K, L, M, and N parameters allowed head-to-head (hh) and head-to-tail (ht) stereoisomers to be distinguished. The different types of hh and ht isomers were assigned on the basis of 3-bond couplings. An example of an A₂B₂ spin system was reported.

L10 ANSWER 31 OF 36 CA COPYRIGHT 2003 ACS

AN 82:154628 CA

TI Photodimers of cinnamic acid and related compounds. Stereochemical study by electron-impact and field desorption mass spectrometry

AU Caccamese, S.; Montaudo, G.; Przybylski, M.

CS Inst. Ind. Chem., Univ. Catania, Catania, Italy

SO Organic Mass Spectrometry (1974), 9(11), 1114-23

CODEN: ORMSBG; ISSN: 0030-493X

DT Journal

LA English

AB The 13 eV electron-impact and field desorption mass spectra of photodimers of cinnamic acid and related compounds containing a cyclobutane ring revealed both sym. and asym. splittings of the ring, thus allowing characterization of the head-to-head and head-to-tail structures of the dimers. A McLafferty type ring opening rearrangement was also observed.

L10 ANSWER 32 OF 36 CA COPYRIGHT 2003 ACS

AN 82:9946 CA

TI Photochemical scission of cinnamic acid dimers. .alpha.-Truxillic and .beta.-truxinic acids

AU Rennert, J.; Grossman, D.
 CS City Coll., City Univ. New York, New York, NY, USA
 SO Journal of Photochemistry (1974), 3(2-3), 163-70
 CODEN: JPCMAE; ISSN: 0047-2670
 DT Journal
 LA English
 AB Excited .alpha.-truxillic acid and .beta.-truxinic acid monomerize in soln. to yield cinnamic acid with quantum efficiencies of 0.12 and 0.41, resp. The photolysis proceeds via excited singlet and triplet mols.

L10 ANSWER 33 OF 36 CA COPYRIGHT 2003 ACS
 AN 78:97032 CA
 TI Structure and conformation of chalcone photodimers and related compounds
 AU Montaudou, G.; Caccamese, S.
 CS Inst. Ind. Chem., Univ. Catania, Catania, Italy
 SO Journal of Organic Chemistry (1973), 38(4), 710-16
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 GI For diagram(s), see printed CA Issue.
 AB Configurational assignments and the conformational preferences of the 2 chalcone (benzalacetophenone) photodimers were reported. Mass spectra and NMR data provided the evidence for the configurational assignments, while dipole moment data and conformational energy ests. were used in the conformational work. Detailed anal. of mass and NMR spectra allowed assignment of the .beta.-truxinic structure to the low melting (m.p. 126.degree.) photodimer (I) and the .alpha.-truxillic structure to the high melting (m.p. 226.degree.) photodimer (II). These results modify previous reports which assigned the .delta.-truxinic structure to the low melting isomer. The conformational properties of these mols. were investigated by comparing the exptl. dipole moments with contour maps of calcd. dipole moments as a function of the internal rotation angles, and with conformational energy maps. These structurally crowded mols. experience drastic restrictions of the conformational space available, so that they exist in well defined, thermodynamically preferred conformations.

L10 ANSWER 34 OF 36 CA COPYRIGHT 2003 ACS
 AN 72:54946 CA
 TI .beta.- and .delta.-Truxinic acids
 AU Freedman, M.; Mohadger, Y.; Rennert, J.; Soloway, S.; Waltcher, I.
 CS City Coll., City Univ. of New York, New York, NY, USA
 SO Organic Preparations and Procedures (1969), 1(4), 267-9
 CODEN: OGPPAC; ISSN: 0375-9512
 DT Journal
 LA English
 AB HO(CH₂)₃OH (38 g), 148 g trans-PhCH:CHCO₂H and 10 g p-MeC₆H₄SO₃H refluxed 3 hr in 150 ml PhMe yielded 85% (PhCH:CHCO₂CH₂)₂CH₂ (I), m. 87-8.degree. (MeOH), with characteristic ir spectrum. I (3 g) refluxed 1 week in 300 ml C₆H₁₂ under irradiation from a 275 W-sun-lamp and the soln. cooled gave 0.2 g bridged cyclobutane diester (II), which was saponified and acidified to yield .delta.-truxinic acid quant. The C₆H₁₂ filtrate evaporated and the oily residue triturated with 10 ml 1:1 Et₂O-petroleum ether gave 1.7 g II isomer (III), C₂₁H₂₀O₄, m. 162-3.degree., characterized by ir spectrum. Saponification of III gave a quant. yield of .beta.-truxinic acid. The overall yield of II and III was 63%.

L10 ANSWER 35 OF 36 CA COPYRIGHT 2003 ACS
 AN 69:86735 CA
 TI Acetylcholine. XII. 3,4-Diphenylthiophene-2,5-dicarboxylic acid bis [(beta.-diethylamino)ethyl ester methiodide], a curarelike muscle-relaxant ester
 AU Dann, O.; Bamberg, K. J.; Sucker, H.
 CS Univ. Erlangen-Nuernberg, Erlangen-Nuernberg, Fed. Rep. Ger.
 SO Pharmazie (1968), 23(3), 135-45
 CODEN: PHARAT; ISSN: 0031-7144
 DT Journal

LA German

GI For diagram(s), see printed CA Issue.

AB The muscle-relaxing properties of quaternized amino alc. esters of 3,4-diphenyl- (I), 3,4-dimethyl- (II), 3,4-di(2-furyl)- (III), and 3,4-bis(5-nitro-2-furyl)thiophene-2,5-dicarboxylic acid (IV); phenanthreno[9,10-c]thiophene-1,3-dicarboxylic acid (V); and 2,3-diphenylbenzene-1,4- (VI), 3,6-diphenylbenzene-1,2- (VII), and 2,5-diphenylfuran-3,4-dicarboxylic acid (VIII) were detd. I (10 g.) was boiled with 300 ml. SOCl_2 and worked up to give 8.1 g. I dichloride (IX), m. 123-4.degree.. Similarly prepd. were 37% II dichloride (X), m. 67-73.degree.; III dichloride (XI), 91%, m. 90.5-1.5.degree. (ligroine); IV dichloride, m. 92.5-95.degree. (C_6H_6); V dichloride (XII), 37%, m. 193-4.degree. (C_6H_6); and VI dichloride (XIII), 80%, m. 153.5-56.degree. (decompn.) (ligroine). VIII (5.5 g.) was added in small portions with stirring to an ice-cold suspension of 16 g. PCl_5 in 55 ml. Et_2O , stirred 30 min., and worked up to give 4.8 g. VIII dichloride (XIV), m. 120-1.degree. (twice from ligroine). Crude II in dioxane was treated with CH_2N_2 in Et_2O , kept 3 hrs., and worked up to give 36% di-Me ester, m. 171.5-2.5.degree. (also prepd. by heating X and MeOH), which was refluxed in methanolic KOH and worked up to give pure II, decomp. 324-7.degree.. Similarly, III (at -5.degree.), gave 90% di-Me ester, m. 129.degree. (twice from AcOH), which, at -5.degree. in Ac_2O , was nitrated with HNO_3 (d. 1.52), stirred 1 hr., and worked up to give IV di-Me ester, m. 182-4.degree., which refluxed 2 min. in methanolic KOH and worked up gave IV, m. 258.degree. (decompn.). A suspension of 2 g. 1,4-dimethyl-2,3-diphenylbenzene in 60 ml. $\text{C}_5\text{H}_5\text{N}$ and 20 ml. H_2O contg. 25.3 g. KMnO_4 was refluxed 2 hrs. and worked up to give 2.2 g. VI, m. 308-11.degree.. IX (15.6 g.) and 25.2 g. .beta.-diethylaminoethanol (DEAE) was refluxed 6 hrs. in 500 ml. dry C_6H_6 and worked up to give 14.8 g. I bis(.beta.-diethylaminoethyl ester), m. 76.5-77.degree. (ligroine); dipicrate m. 175.5-77.degree. (1:1 $\text{Me}_2\text{CO}-\text{H}_2\text{O}$); di-HBr salt m. 185.5-6.5.degree. ($\text{Me}_2\text{CO}-\text{iso-PrOH}$); dimethiodide m. 212-13.degree. (decompn.); bis(benzyl bromide) decompd. 191.degree., m. 240-7.degree. ($\text{EtOH}-\text{EtOAc}$). The following were prepd. II bis(.beta.-diethylaminoethyl ester), 70% [di-HBr salt m. 212.5-14.degree. (decompn.); dimethiodide m. 202.5-2.5.degree. (decompn.)]; III bis(.beta.-diethylaminoethyl ester), 61%, n22D 1.459, by shaking XI and DEAE in C_6H_6 66 hrs. at room temp. and working up [di-HBr salt, m. 179.5-81.degree. (decompn.); dimethiodide m. 177.5-79.degree. (decompn.)]; IV bis(.beta.-diethylaminoethyl ester), 47%, m. 42-7.degree. (dimethiodide m. 192-5.degree.); VI bis(.beta.-diethylaminoethyl ester), 62%, n22D 1.540 [di-HBr salt m. 185.5-7.5.degree. ($\text{EtOAc}:\text{EtOH}$); dimethiodide, m. 234-5.degree. (decompn.)]; VIII bis(.beta.-diethylaminoethyl ester), 74% [di-HBr salt m. 180-1.degree. (3:1 $\text{Me}_2\text{CO}-\text{EtOH}$); dimethiodide m. 185.5-87.degree. (decompn.)] I bis(.beta.-dimethylaminoethyl ester). 65%, m. 69-79.degree. (ligroine) [dimethiodide decompd. 225-50.degree. (EtOH)]; and V bis(.beta.-diethylaminoethyl ester), 90%, [di-HCl salt, decomp. 211-12.5.degree.; dimethiodide m. 215-16.degree. (decompn.)]. XII (1.25 g.) and 1.1 g. MeOH refluxed in 5 ml. C_6H_6 and cooled pptd. 0.85 g. V di-Me ester, m. 118-19.degree.. DEAE (4.7 g.) in 50 ml. Me_2CO was added to 12 g. VII anhydride suspended in 250 ml. dry refluxing Me_2CO , and the mixt. refluxed 20 min. to ppt. 14.6 g. of the half ester, m. 205-22.degree., difficulty sol. in 2N NaOH and 2N HCl. This intermediate (8.35 g.) and 5.4 g. .beta.-diethylaminoethyl chloride was refluxed 6.5 hrs. in 160 ml. dry iso-PrOH and worked up to give 7.3 g. VII bis(.beta.-diethylaminoethyl ester), m. 99-100.degree. (ligroine and petroleum ether); di-HBr salt m. 193-5.degree.; dimethiodide m. 206.5-7.5.degree. (decompn.). The anhydride (5 g.) of cis, cis, cis, cis-3,6-diphenyl-1,2,3,6-tetrahydrobenzene-1,2-dicarboxylic acid in 80 ml. HCONMe_2 was hydrogenated at atm. pressure and room temp. over $\text{Pd}(\text{OH})_2$ on BaSO_4 and worked up to give 3.3 g. anhydride of cis, cis, cis, cis-3,6-diphenylcyclohexane-1,2-dicarboxylic acid, m. 220-2.degree. (EtOAc). A soln. of 4.8 g. 2,7-diaminodiphenylene sulfone and 14 g. di-Et diacetylsuccinate in 20 ml. AcOH was refluxed 45 min. and cooled to ppt. 12.5 g. XV, m. 251-3.degree. ($\text{BuOH}:\text{AcOH}$), sapond. to the free acid by methanolic KOH. A mixt. of 1.28 g. 2,2'-dihydroxy-5,5'-dimethyldeoxybenzoin in 2N NaOH and 1 g. $\text{ClCH}_2\text{CO}_2\text{H}$ soln. neutralized with

K₂CO₃ was refluxed 3 hrs. and worked up to give 2-hydroxy-2'-carboxymethoxy-5,5'-dimethyldeoxybenzoin, m. 159-61.degree. (60% EtOH), and 2,2'-dicarboxymethoxy-5,5'-dimethyldeoxybenzoin, m. 172-4.degree. (60% AcOH and 60% EtOH). Extensive biol. data are given.

L10 ANSWER 36 OF 36 CA COPYRIGHT 2003 ACS

AN 66:82172 CA

TI Separation of trans-cinnamic, .alpha.-truxillic, and .beta.-truxinic acids by paper chromatography

AU Sonntag, Friedrich I.

CS IBM Watson Res. Center, Yorktown Heights, NY, USA

SO Journal of Chromatography (1967), 26(2), 544

CODEN: JOCRAM; ISSN: 0021-9673

DT Journal

LA English

AB The title acids were sepd. by chromatog. on Whatman No. 1 paper. EtOH-H₂O-NH₄OH (80:10:5) was used as solvent for a front migration of 30 cm. The sheets were dried, and sprayed with a mixt. of 300 mg. bromothymol blue and 0.25 ml. 30% aq. NaOH in 500 ml. EtOH. Rf values were cinnamic acid, 0.56; .alpha.-truxillic acid, 0.36; .beta.-truxinic acid, 0.27. Cl- had to be excluded from the mixt.

=>

=> FIL STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

95.24

414.21

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-22.32

-24.18

FILE 'STNGUIDE' ENTERED AT 14:49:44 ON 21 APR 2003

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE

AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Apr 18, 2003 (20030418/UP).

=>